Materials and Methods. All reactions involving metal complexes were conducted in oven-dried glassware under an argon atmosphere using standard Schlenk techniques and anhydrous solvents obtained from Sigma-Aldrich. All commercial reagents were used as received. Ruthenium complexes **1**[1] and **3**[2] as well as the different 2-(3-butenyl)pyridine ligands[3] were prepared according to literature procedures. ^{1}H and ^{13}C NMR spectra were recorded on Varian Mercury 300 Spectrometer (at 300 and 75 MHz, respectively) and the chemical shifts are reported in ppm relative to tetramethylsilane (δ 0.0). X-ray crystallographic structures were obtained by Mr. Larry M. Henling and Dr. Mike W. Day of the California Institute of Technology Beckman Institute X-Ray Crystallography Laboratory.

(sIMes)(Cl)$_2$Ru(CH(CH$_2$)$_2$-*C*,*N*-2-C$_5$H$_4$N)-*C*$_s$ (4a). Method A: A 250 mL round bottom schlenk flask equipped with a stir bar was charged with **1** (10.0 g; 11.8 mmol). The flask was capped, sparged with argon for 15 minutes, and charged with anhydrous CH_2Cl_2 (118 mL) via cannula. 2-(3-Butenyl)pyridine (2.4 g, 17.7 mmol) was then added via syringe and the reaction mixture was heated to 40 °C for 5-6 hours. The reaction mixture was concentrated to dryness and the residue triturated with degassed, chilled methanol. The solid was collected on a frit and washed with chilled methanol (2 x 25 mL) to give **4a** (5.6 g; 9.4 mmol) as a pale green solid upon drying. Yield: 80 %. **Method B:** In the glove box a vial was charged with 2-(3-butenyl)pyridine (24 mg, 0.18 mmol) and CH_2Cl_2 (2 mL). Complex **3** (86 mg; 0.12 mmol) was then added as a solid and the reaction allowed to stir at room temperature for 30 minutes. The volatiles were removed under vacuum and the residue triturated with hexanes. The solid was collected, washed with hexanes (2 x 1 mL) and dried under vacuum to give **4a** (60 mg; 0.10 mmol) as a pale green solid upon drying. Yield: 85 %. ^{1}H NMR (CD_2Cl_2): δ 18.46 (t, $^{3}J_{HH}$ = 2.7 Hz, 1 H, Ru=CH), 7.64 (d, $^{3}J_{HH}$ = 4.8 Hz, 1 H, Py), 7.52 (t, $^{3}J_{HH}$ = 7.2 Hz, 1 H, Py), 7.14 (d, $^{3}J_{HH}$ = 7.8 Hz, 1 H, Py), 7.07 (s, 4 H, Mes), 6.99 (t, $^{3}J_{HH}$ = 6.9 Hz, 1 H, Py), 4.09 (s, 4 H, sIMes), 3.55 (t, $^{3}J_{HH}$ = 5.7 Hz, 2 H, CH_2-Py), 2.50 (s, 12 H, Mes-CH_3), 2.41 (s, 6 H, Mes-CH_3), 1.70 (m, 2 H, Ru=CH-C*H*$_2$). ^{13}C{^{1}H} NMR (CD_2Cl_2): δ 339.18 (Ru=*C*HCH2), 216.52 (Ru-C(N)$_2$), 162.64, 158.34, 149.54, 138.96, 138.83, 136.96, 129.60, 124.51, 121.82, 54.45, 51.92, 34.30, 21.32, 19.58.

(sIMes)(Cl)$_2$Ru(CH(CH$_2$)$_2$-*C*,*N*-2-(4-Me)-C$_5$H$_3$N)-*C*$_s$ (5) In the glove box, a flask was charged with 2-(3-butenyl)-4-methylpyridine (40 mg, 0.27 mmol) and CH_2Cl_2 (5 mL). Complex

1 Scholl, M.; Ding, S.; Lee, C. W.; Grubbs, R. H. Org. Lett. 1999, 1, 953-956.

2 Sanford, M. S.; Love, J. A.; Grubbs, R. H. Organometallics 2001, 20, 5314-5318.

3 van der Schaaf, P. A.; Kolly, R.; Kirner, H.-J.; Rime, F.; Mühlebach, A.; Hafner, A. J. Organomet. Chem. 2000, 606, 65-74.

3 (114 mg; 0.16 mmol) was then added as a solid and the reaction allowed to stir at room temperature for 30 minutes. The volatiles were removed under vacuum and the residue was redissolved in C_6H_6 (1 mL) and precipitated with pentane (10 mL). The solid was collected, washed with pentane (3 x 5 mL) and dried under vacuum to give **5** (80 mg; 0.13 mmol) as a light brown solid upon drying. Yield: 84 %. ^{1}H NMR (CD_2Cl_2): δ 18.44 (t, $^3J_{HH}$ = 3.3 Hz, 1 H, Ru=CH), 7.42 (d, $^3J_{HH}$ = 5.7 Hz, 1 H, Py), 7.02 (s, 4 H, Mes), 6.95 (s, 1 H, Py), 6.80 (d, $^3J_{HH}$ = 4.2 Hz, 1 H, Py), 4.06 (s, 4 H, sIMes), 3.46 (t, $^3J_{HH}$ = 6.0 Hz, 2 H, CH_2-Py), 2.45 (s, 12 H, Mes-CH_3), 2.37 (s, 6 H, Mes-CH_3), 2.27 (s, 3 H, Py-CH_3), 1.66 (m, 2 H, Ru=CH-CH_2). ^{13}C{^{1}H} NMR (CD_2Cl_2): δ 339.16 (Ru=*C*HCH2), 216.91 (Ru-C$(N)_2$), 161.97, 148.96, 148.87, 138.99, 138.83, 129.63, 125.43, 122.98, 54.62, 51.95, 34.13, 21.35, 21.01, 19.64.

(sIMes)(Cl)$_2$Ru(CH(CH$_2$)$_2$-*C*,*N*-2-(6-Me)-C$_5$H$_3$N)-*C*$_s$ (6). In the glove box, a flask was charged with 2-(3-butenyl)-6-methylpyridine (50 mg, 0.34 mmol) and CH_2Cl_2 (5 mL). Complex **3** (98 mg; 0.14 mmol) was then added as a solid and the reaction allowed to stir at room temperature for 30 minutes. The volatiles were removed under vacuum and the residue was redissolved in C_6H_6 (1 mL) and precipitated with pentane (10 mL). The solid was collected, washed with pentane (3 x 5 mL) and dried under vacuum to give **6** (57 mg; 0.094 mmol) as a light brown solid upon drying. Yield: 69 %. ^{1}H NMR (CD_2Cl_2): δ 18.33 (t, $^3J_{HH}$ = 3.6 Hz, 1 H, Ru=CH), 7.34 (t, $^3J_{HH}$ = 7.5 Hz, 1 H, Py), 7.03 (s, 4 H, Mes), 6.97 (d, $^3J_{HH}$ = 7.8 Hz, 1 H, Py), 6.75 (d, $^3J_{HH}$ = 7.8 Hz, 1 H, Py), 4.05 (m, 4 H, sIMes), 2.91 (m, 4 H, Ru=CH-CH_2-CH_2-Py), 2.61 (br s, 6 H, Mes-CH_3), 2.37 (s, 6 H, Mes-CH_3), 2.31 (br s, 6 H, Mes-CH_3), 2.01 (s, 3 H, Py-CH_3). ^{13}C{^{1}H} NMR (CD_2Cl_2): δ 343.54 (Ru=*C*HCH2), 218.21 (Ru-C$(N)_2$), 160.62, 160.55, 140.45, 139.29, 138.73, 137.88, 136.65, 129.79, 128.82, 123.03, 122.13, 52.04, 51.24, 34.66, 32.20, 22.86, 21.76, 21.34, 20.37, 18.51.

(sIMes)(Cl)$_2$Ru(CH(CH$_2$)$_2$-*C*,*N*-2-C$_5$H$_4$N)-*C*$_1$ (4b). A 220 mL round bottom Schlenk flask equipped with a stir bar was charged with complex **1** (5.0 g; 5.9 mmol). The flask was capped, sparged with argon for 15 minutes, and charged with anhydrous CH_2Cl_2 (60 mL) via cannula. 2-(3-Butenyl)pyridine (1.2 g, 8.9 mmol) was then added via syringe and the reaction mixture was heated to 40 °C for 3-4 days. The reaction mixture was concentrated to dryness and the residue triturated with degassed, chilled methanol (15 mL). The solid was collected on a frit and washed with methanol (2 x 10 mL) to give **4b** (1.3 g; 2.2 mmol) as an orange-brown solid upon drying. Yield: 37 %. ^{1}H NMR (CD_2Cl_2): δ 19.14 (t, $^3J_{HH}$ = 3.3 Hz, 1 H, Ru=CH), 7.54 (d, $^3J_{HH}$ = 7.8 Hz, 1 H, Py), 7.49 (t, $^3J_{HH}$ = 5.1 Hz, 1 H, Py), 7.25 (s, 1 H, Mes), 7.06 (s, 1 H, Mes),

7.03 (d, $^3J_{HH}$ = 7.8 Hz, 1 H, Py), 6.90 (s, 1 H, Mes), 6.88 (s, 1 H, Mes), 6.81 (t, $^3J_{HH}$ = 6.6 Hz, 1 H, Py), 4.15 (m, 2 H, sIMes), 3.90 (m, 2 H, sIMes), 3.00 (m, 2 H, CH_2-Py), 2.88 (s, 3 H, Mes-CH_3), 2.69 (s, 3 H, Mes-CH_3), 2.40 (s, 3 H, Mes-CH_3), 2.34 (s, 3 H, Mes-CH_3), 1.96 (s, 3 H, Mes-CH_3), 1.78 (m, 1 H, Ru=CH-CH_2), 1.45 (s, 3 H, Mes-CH_3), 1.21 (m, 1 H, Ru=CH-CH_2). $^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ 319.04 (Ru=*C*HCH2), 218.94 (Ru-C$(N)_2$), 161.71, 154.02, 139.51, 138.94, 138.32, 137.90, 135.57, 134.97, 132.96, 130.26, 129.53, 129.34, 129.16, 128.65, 122.94, 120.00, 50.54, 49.23, 34.87, 20.52, 20.27, 19.25, 18.92, 18.39, 17.56.

Conversion of 4a to 4b. In the glove box, a 0.1 M solution of **4a** in CD_2Cl_2 was prepared and transferred to an NMR tube, which was capped and taken out of the glove box. The NMR tube was left in an oil bath at 40 °C and the reaction was monitored by ^1H NMR spectroscopy. The composition of the mixture was the following **4b**/**4a** = 30/70 after 24 hours; 60/40 after 48 hours; 70/30 after 72 hours; and 78/22 after 96 hours.

Conversion of 4b to 4a. In the glove box, a 0.1 M solution of **4b** in CD_2Cl_2 was prepared and transferred to an NMR tube, which was capped and taken out of the glove box. The NMR tube was left in an oil bath at 40 °C and the reaction was monitored by ^1H NMR spectroscopy. The composition of the mixture was the following **4b**/**4a** = 83/17 after 24 hours. ^1H NMR spectroscopy also showed that the isomerization of **4b** was accompanied with some catalyst decomposition, making it complicated to analyze the reaction mixture beyond 24 hours.

RCM of Diethyldiallyl Malonate. The ring-closing metathesis of diethyldiallyl malonate was used as a test reaction to compare the activity of catalysts **1**, **4a** and **4b** on one hand and **4a**, **5** and **6** on the other hand. For the comparison of **1**, **4a** and **4b**: 1 mol % of catalyst was added to a 0.1 M solution of diethyldiallyl malonate in dichloromethane and the reaction was allowed to proceed at 25 °C and was monitored by gas-chromatography (Figure 1). For the comparison of **4a**, **5** and **6**: in the dry box, 2.5 mol % of catalyst (0.0052 mmol) was dissolved in C_6D_6 (0.65 mL) in an NMR tube fitted with a teflon septum screw-cap. The resulting solution was allowed to equilibrate in the NMR probe at 40 ºC. Diethyl diallylmalonate (50 μL, 0.207 mmol, 0.30 M) was injected into the NMR tube neat and the reaction was monitored by ^1H NMR spectroscopy. The olefinic resonances integrals of the product relative to that of the starting material were measured with the residual protio solvent peak used as an internal standard (Figure 2).

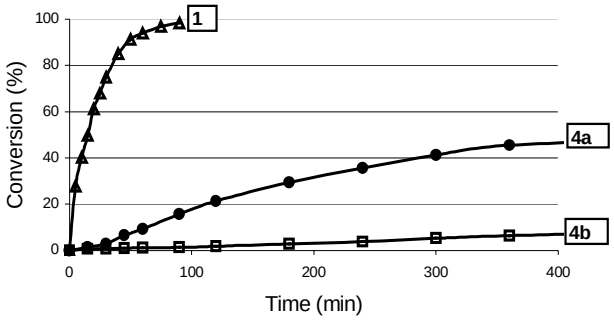


Figure 1. RCM of diethyl diallylmalonate in CH_2Cl_2 (0.1 M) at 25 °C using **1**, **4a** and **4b** (1 mol %).

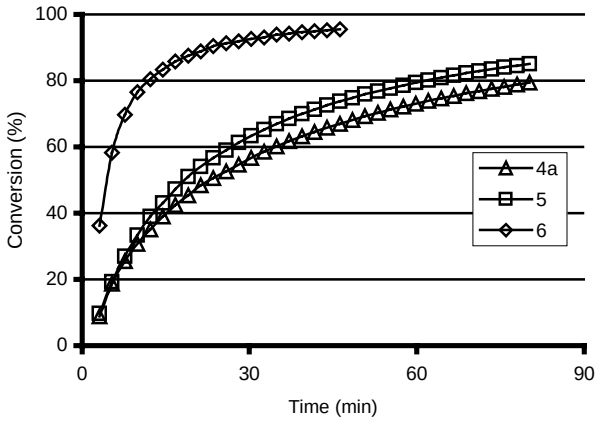


Figure 2. RCM of diethyl diallylmalonate in CH_2Cl_2 (0.3 M) at 40 °C using **4a**, **5** and **6** (2.5 mol %).

ROMP of DCPD. Dicyclopentadiene containing 3.5% of tricyclopentadiene (100 g) was polymerized by addition of catalyst (monomer/catalyst = 30,000 or 40,000) at 30 °C. The reaction was monitored by measuring the polymerization exotherm.

Table 1. Crystal data and structure refinement for 4a.

Empirical formula	$C_{29}H_{35}Cl_2N_3Ru$
Formula weight	597.57
Crystallization Solvent	Benzene/hexane
Crystal Habit	Block
Crystal size	0.33 x 0.32 x 0.14 mm^3
Crystal color	Dark brown

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	Bruker SMART 1000	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 26248 reflections used in lattice determination	2.22 to 44.64°	
Unit cell dimensions	a = 8.5295(2) Å b = 11.8164(2) Å c = 13.9583(3) Å	α= 84.9350(10)° β= 81.3450(10)° γ = 80.0880(10)°
Volume	1367.23(5) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.452 Mg/m^3	
F(000)	616	
Data collection program	Bruker SMART v5.054	
θ range for data collection	1.75 to 45.08°	
Completeness to θ = 45.08°	93.6 %	
Index ranges	$-16 \le h \le 16, -23 \le k \le 23, -27 \le l \le 27$	

Data collection scan type	ω scans at 9 ϕ settings
Data reduction program	Bruker SAINT v6.45
Reflections collected	57225
Independent reflections	21200 [R_{int}= 0.0666]
Absorption coefficient	0.791 mm^{-1}
Absorption correction	None
Max. and min. transmission (predicted)	0.8973 and 0.7802

Table 1 (cont.)

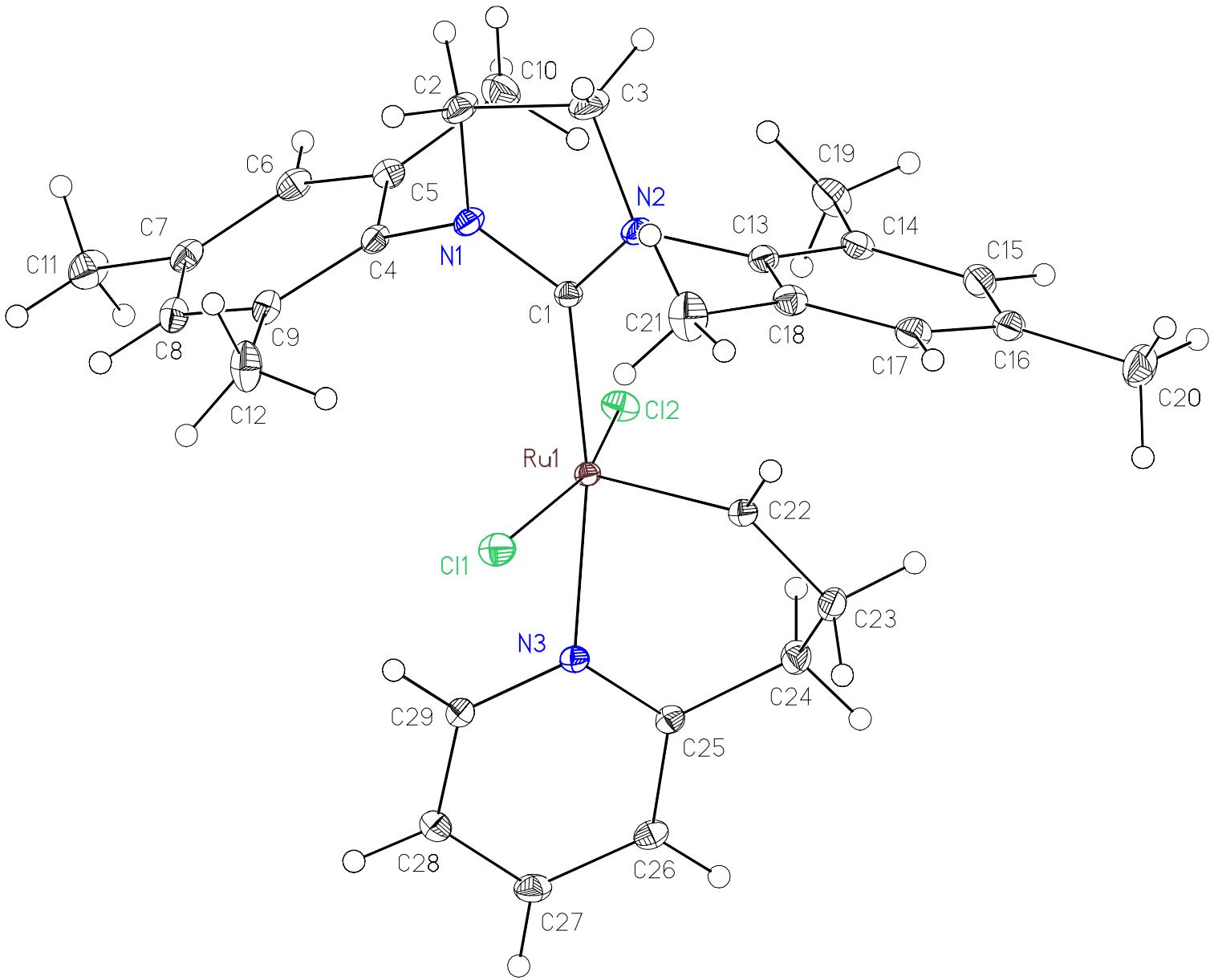
Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	21200 / 0 / 322
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.263
Final R indices [I>2σ(I), 15876 reflections]	R1 = 0.0382, *w*R2 = 0.0751
R indices (all data)	R1 = 0.0589, *w*R2 = 0.0782
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.003
Average shift/error	0.000
Largest diff. peak and hole	1.881 and -1.273 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C2
C10
C3
C6
C5
C19
N2
C7
N1
C13
C14
C15
C11
C4
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C18
C8
C9
C17
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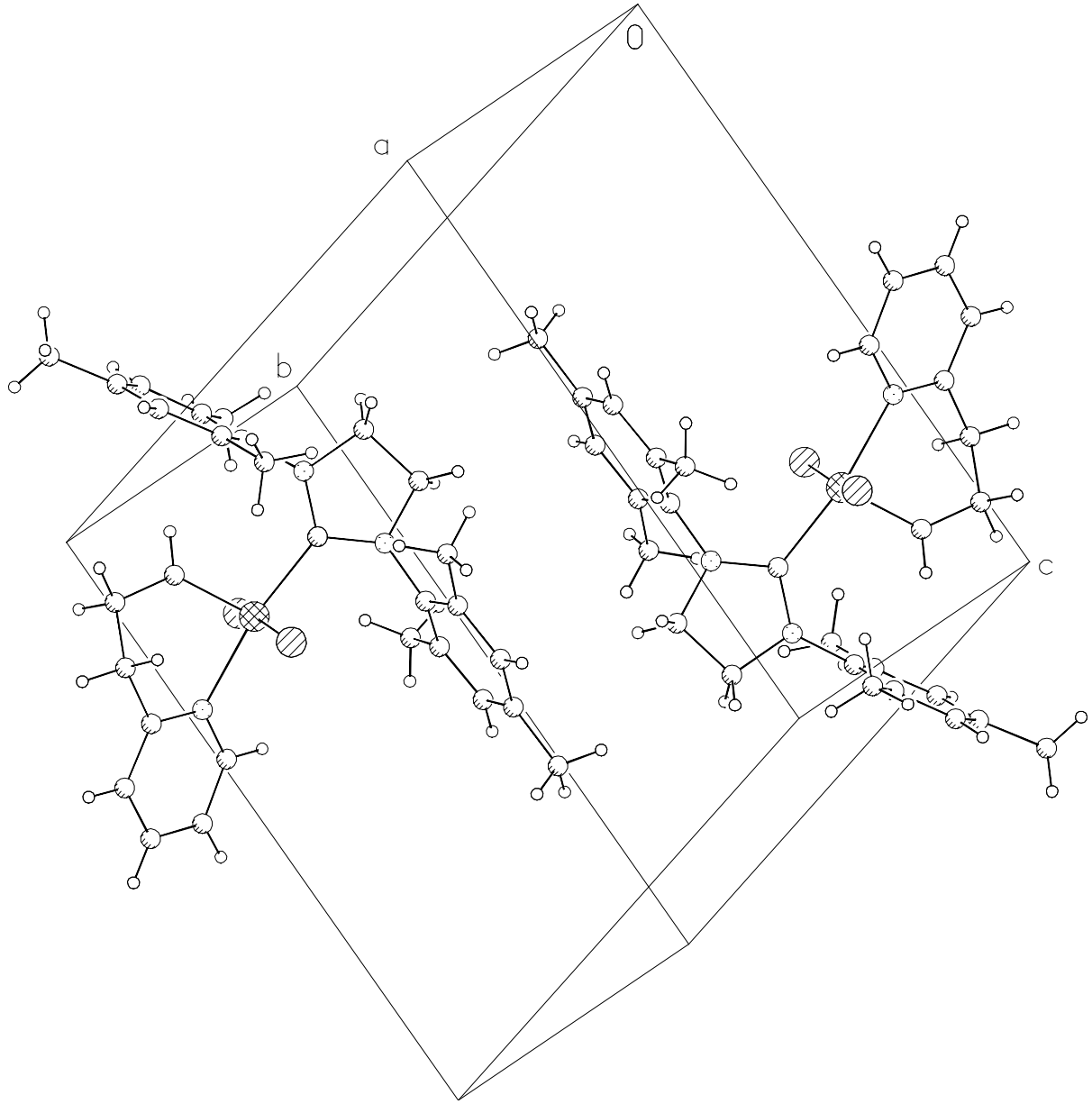
C23
N3
C24
C29
C25
C28
C26
C27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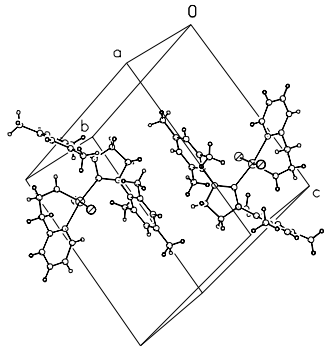
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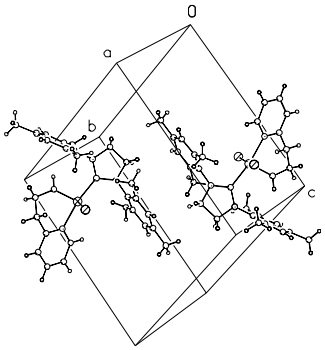

0
a
b
c

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 4a. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	8734(1)	8476(1)	2729(1)	8(1)
Cl(1)	6564(1)	9914(1)	2297(1)	14(1)
Cl(2)	10528(1)	7160(1)	3587(1)	12(1)
N(1)	6532(1)	6718(1)	3234(1)	11(1)
N(2)	7209(1)	6841(1)	1666(1)	12(1)
N(3)	9803(1)	9804(1)	3192(1)	9(1)
C(1)	7466(1)	7223(1)	2510(1)	9(1)
C(2)	5447(2)	6049(1)	2882(1)	15(1)
C(3)	6152(2)	5963(1)	1816(1)	19(1)
C(4)	6485(1)	6741(1)	4268(1)	10(1)
C(5)	7329(1)	5798(1)	4758(1)	12(1)
C(6)	7201(1)	5781(1)	5768(1)	13(1)
C(7)	6238(1)	6662(1)	6292(1)	12(1)
C(8)	5367(1)	7562(1)	5788(1)	12(1)
C(9)	5462(1)	7613(1)	4775(1)	11(1)
C(10)	8338(2)	4810(1)	4227(1)	19(1)
C(11)	6176(2)	6643(1)	7378(1)	18(1)
C(12)	4429(1)	8561(1)	4260(1)	18(1)
C(13)	8222(1)	6932(1)	757(1)	11(1)
C(14)	9799(1)	6333(1)	658(1)	12(1)
C(15)	10792(1)	6498(1)	-220(1)	14(1)
C(16)	10242(1)	7203(1)	-991(1)	14(1)
C(17)	8636(2)	7742(1)	-880(1)	14(1)
C(18)	7613(1)	7623(1)	-13(1)	12(1)
C(19)	10462(2)	5560(1)	1467(1)	17(1)
C(20)	11336(2)	7385(1)	-1924(1)	21(1)
C(21)	5920(2)	8275(1)	101(1)	21(1)
C(22)	9861(1)	8679(1)	1530(1)	10(1)
C(23)	11452(1)	9078(1)	1300(1)	14(1)
C(24)	12324(1)	9174(1)	2163(1)	13(1)
C(25)	11354(1)	9937(1)	2916(1)	10(1)
C(26)	12012(1)	10746(1)	3328(1)	12(1)
C(27)	11080(1)	11424(1)	4034(1)	14(1)
C(28)	9484(1)	11294(1)	4301(1)	13(1)
C(29)	8900(1)	10480(1)	3866(1)	11(1)

Table 3. Selected bond lengths [Å] and angles [°] for 4a.

Ru(1)-C(22)	1.8185(11)	C(22)-Ru(1)-C(1)	101.35(4)
Ru(1)-C(1)	2.0459(10)	C(22)-Ru(1)-N(3)	88.32(4)
Ru(1)-N(3)	2.1355(9)	C(1)-Ru(1)-N(3)	170.21(4)
Ru(1)-Cl(2)	2.3662(3)	C(22)-Ru(1)-Cl(2)	104.21(3)
Ru(1)-Cl(1)	2.3973(3)	C(1)-Ru(1)-Cl(2)	92.32(3)
		N(3)-Ru(1)-Cl(2)	86.74(2)
		C(22)-Ru(1)-Cl(1)	90.58(3)
		C(1)-Ru(1)-Cl(1)	89.52(3)
		N(3)-Ru(1)-Cl(1)	88.82(2)
		Cl(2)-Ru(1)-Cl(1)	164.406(11)

Table 4. Bond lengths [Å] and angles [°] for 4a.

Ru(1)-C(22)	1.8185(11)	C(1)-N(2)-C(3)	113.02(9)
Ru(1)-C(1)	2.0459(10)	C(13)-N(2)-C(3)	118.74(9)
Ru(1)-N(3)	2.1355(9)	C(29)-N(3)-C(25)	118.75(9)
Ru(1)-Cl(2)	2.3662(3)	C(29)-N(3)-Ru(1)	116.94(7)
Ru(1)-Cl(1)	2.3973(3)	C(25)-N(3)-Ru(1)	124.04(7)
N(1)-C(1)	1.3514(13)	N(1)-C(1)-N(2)	106.82(8)
N(1)-C(4)	1.4408(13)	N(1)-C(1)-Ru(1)	123.04(7)
N(1)-C(2)	1.4765(14)	N(2)-C(1)-Ru(1)	129.65(8)
N(2)-C(1)	1.3591(13)	N(1)-C(2)-C(3)	101.80(9)
N(2)-C(13)	1.4296(14)	N(2)-C(3)-C(2)	102.52(9)
N(2)-C(3)	1.4693(14)	C(5)-C(4)-C(9)	121.27(10)
N(3)-C(29)	1.3487(14)	C(5)-C(4)-N(1)	118.07(10)
N(3)-C(25)	1.3527(13)	C(9)-C(4)-N(1)	120.18(10)
C(2)-C(3)	1.5234(16)	C(6)-C(5)-C(4)	118.28(10)
C(4)-C(5)	1.4024(15)	C(6)-C(5)-C(10)	119.85(10)
C(4)-C(9)	1.3989(15)	C(4)-C(5)-C(10)	121.87(10)
C(5)-C(6)	1.3961(16)	C(5)-C(6)-C(7)	121.70(10)
C(5)-C(10)	1.5060(16)	C(8)-C(7)-C(6)	118.55(10)
C(6)-C(7)	1.3982(16)	C(8)-C(7)-C(11)	121.02(11)
C(7)-C(8)	1.3895(15)	C(6)-C(7)-C(11)	120.42(10)
C(7)-C(11)	1.5073(15)	C(7)-C(8)-C(9)	121.58(10)
C(8)-C(9)	1.4002(15)	C(8)-C(9)-C(4)	118.50(10)
C(9)-C(12)	1.5024(15)	C(8)-C(9)-C(12)	120.07(10)
C(13)-C(18)	1.3995(15)	C(4)-C(9)-C(12)	121.37(10)
C(13)-C(14)	1.4015(16)	C(18)-C(13)-C(14)	121.48(10)
C(14)-C(15)	1.3993(16)	C(18)-C(13)-N(2)	119.08(10)
C(14)-C(19)	1.5038(16)	C(14)-C(13)-N(2)	119.44(10)
C(15)-C(16)	1.3900(16)	C(15)-C(14)-C(13)	118.05(10)
C(16)-C(17)	1.4001(17)	C(15)-C(14)-C(19)	119.58(11)
C(16)-C(20)	1.5050(16)	C(13)-C(14)-C(19)	122.34(10)
C(17)-C(18)	1.3934(16)	C(16)-C(15)-C(14)	121.99(11)
C(18)-C(21)	1.5078(16)	C(15)-C(16)-C(17)	118.24(10)
C(22)-C(23)	1.4931(15)	C(15)-C(16)-C(20)	121.21(11)
C(23)-C(24)	1.5297(16)	C(17)-C(16)-C(20)	120.55(11)
C(24)-C(25)	1.5009(15)	C(18)-C(17)-C(16)	121.75(10)
C(25)-C(26)	1.3925(14)	C(17)-C(18)-C(13)	118.38(10)
C(26)-C(27)	1.3889(16)	C(17)-C(18)-C(21)	120.26(10)
C(27)-C(28)	1.3871(16)	C(13)-C(18)-C(21)	121.29(10)
C(28)-C(29)	1.3791(15)	C(23)-C(22)-Ru(1)	126.75(8)
		C(22)-C(23)-C(24)	116.50(9)
C(22)-Ru(1)-C(1)	101.35(4)	C(25)-C(24)-C(23)	113.77(9)
C(22)-Ru(1)-N(3)	88.32(4)	N(3)-C(25)-C(26)	120.68(10)
C(1)-Ru(1)-N(3)	170.21(4)	N(3)-C(25)-C(24)	117.38(9)
C(22)-Ru(1)-Cl(2)	104.21(3)	C(26)-C(25)-C(24)	121.93(9)
C(1)-Ru(1)-Cl(2)	92.32(3)	C(27)-C(26)-C(25)	120.13(10)
N(3)-Ru(1)-Cl(2)	86.74(2)	C(28)-C(27)-C(26)	118.74(10)
C(22)-Ru(1)-Cl(1)	90.58(3)	C(29)-C(28)-C(27)	118.45(10)
C(1)-Ru(1)-Cl(1)	89.52(3)	N(3)-C(29)-C(28)	123.22(10)
N(3)-Ru(1)-Cl(1)	88.82(2)		
Cl(2)-Ru(1)-Cl(1)	164.406(11)		
C(1)-N(1)-C(4)	128.85(9)		
C(1)-N(1)-C(2)	113.33(9)		
C(4)-N(1)-C(2)	117.82(9)		
C(1)-N(2)-C(13)	124.94(9)		

Table 5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for 4a. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	80(1)	74(1)	75(1)	-5(1)	-10(1)	-22(1)
Cl(1)	95(1)	120(1)	198(1)	-4(1)	-35(1)	-11(1)
Cl(2)	162(1)	100(1)	118(1)	8(1)	-57(1)	-16(1)
N(1)	128(4)	132(4)	82(3)	-5(3)	-7(3)	-70(3)
N(2)	150(4)	130(4)	88(3)	-18(3)	-5(3)	-78(3)
N(3)	92(3)	88(3)	100(3)	-6(3)	-18(3)	-21(3)
C(1)	95(4)	87(4)	92(4)	-8(3)	-14(3)	-24(3)
C(2)	168(5)	184(5)	122(4)	-10(4)	-11(4)	-110(4)
C(3)	252(6)	213(5)	132(5)	-31(4)	-11(4)	-160(5)
C(4)	107(4)	121(4)	86(4)	2(3)	-7(3)	-44(3)
C(5)	137(4)	105(4)	123(4)	5(3)	-5(3)	-30(3)
C(6)	144(4)	131(4)	123(4)	34(3)	-23(3)	-41(3)
C(7)	124(4)	162(5)	95(4)	16(3)	-24(3)	-63(3)
C(8)	109(4)	162(5)	101(4)	-10(3)	-7(3)	-28(3)
C(9)	93(4)	146(4)	100(4)	4(3)	-10(3)	-24(3)
C(10)	224(6)	132(5)	184(5)	-15(4)	-11(4)	-3(4)
C(11)	225(6)	216(6)	105(5)	21(4)	-44(4)	-82(4)
C(12)	145(5)	244(6)	123(5)	21(4)	-5(4)	52(4)
C(13)	149(4)	105(4)	85(4)	-9(3)	-9(3)	-45(3)
C(14)	176(5)	89(4)	98(4)	-8(3)	-26(3)	-20(3)
C(15)	153(5)	124(4)	129(4)	-22(3)	-10(3)	-13(3)
C(16)	192(5)	116(4)	106(4)	-10(3)	5(3)	-46(4)
C(17)	198(5)	110(4)	103(4)	5(3)	-31(4)	-34(4)
C(18)	152(4)	123(4)	109(4)	-9(3)	-36(3)	-34(3)
C(19)	242(6)	133(5)	123(5)	-4(4)	-46(4)	14(4)
C(20)	234(6)	210(6)	155(5)	28(4)	44(4)	-42(5)
C(21)	173(5)	252(6)	176(5)	2(5)	-40(4)	21(4)
C(22)	113(4)	99(4)	105(4)	-12(3)	-7(3)	-32(3)
C(23)	127(4)	167(5)	118(4)	-28(4)	16(3)	-58(4)
C(24)	91(4)	156(5)	143(5)	-32(4)	-7(3)	-25(3)
C(25)	85(4)	97(4)	106(4)	6(3)	-19(3)	-17(3)
C(26)	110(4)	123(4)	132(4)	7(3)	-36(3)	-43(3)
C(27)	166(5)	128(4)	136(5)	-13(3)	-39(4)	-64(4)
C(28)	155(5)	124(4)	124(4)	-32(3)	-6(3)	-33(3)
C(29)	110(4)	112(4)	108(4)	-11(3)	0(3)	-31(3)

Table 6. Crystal data and structure refinement for 4b.

Empirical formula	$C_{29}H_{35}Cl_2N_3Ru \cdot CH_2Cl_2$
Formula weight	682.50
Crystallization Solvent	Dichloromethane
Crystal Habit	Block
Crystal size	0.37 x 0.32 x 0.18 mm^3
Crystal color	Pale orange/brown

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 21345 reflections used in lattice determination	2.22 to 28.35°
Unit cell dimensions	a = 8.7869(4) Å b = 14.1539(7) Å β= 93.7840(10)° c = 23.9944(12) Å
Volume	2977.7(2) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.522 Mg/m^3
F(000)	1400
Data collection program	Bruker SMART v5.054
θ range for data collection	1.67 to 28.38°
Completeness to θ = 28.38°	93.3 %
Index ranges	$-11 \le h \le 11$, $-18 \le k \le 18$, $-31 \le l \le 31$
Data collection scan type	ω scans at 4 ϕ settings and 1 ϕ scan
Data reduction program	Bruker SAINT v6.022
Reflections collected	47818
Independent reflections	6963 [R_{int}= 0.0639]
Absorption coefficient	0.911 mm^{-1}
Absorption correction	None
Max. and min. transmission (predicted)	0.8532 and 0.7293

Table 6 (cont.)

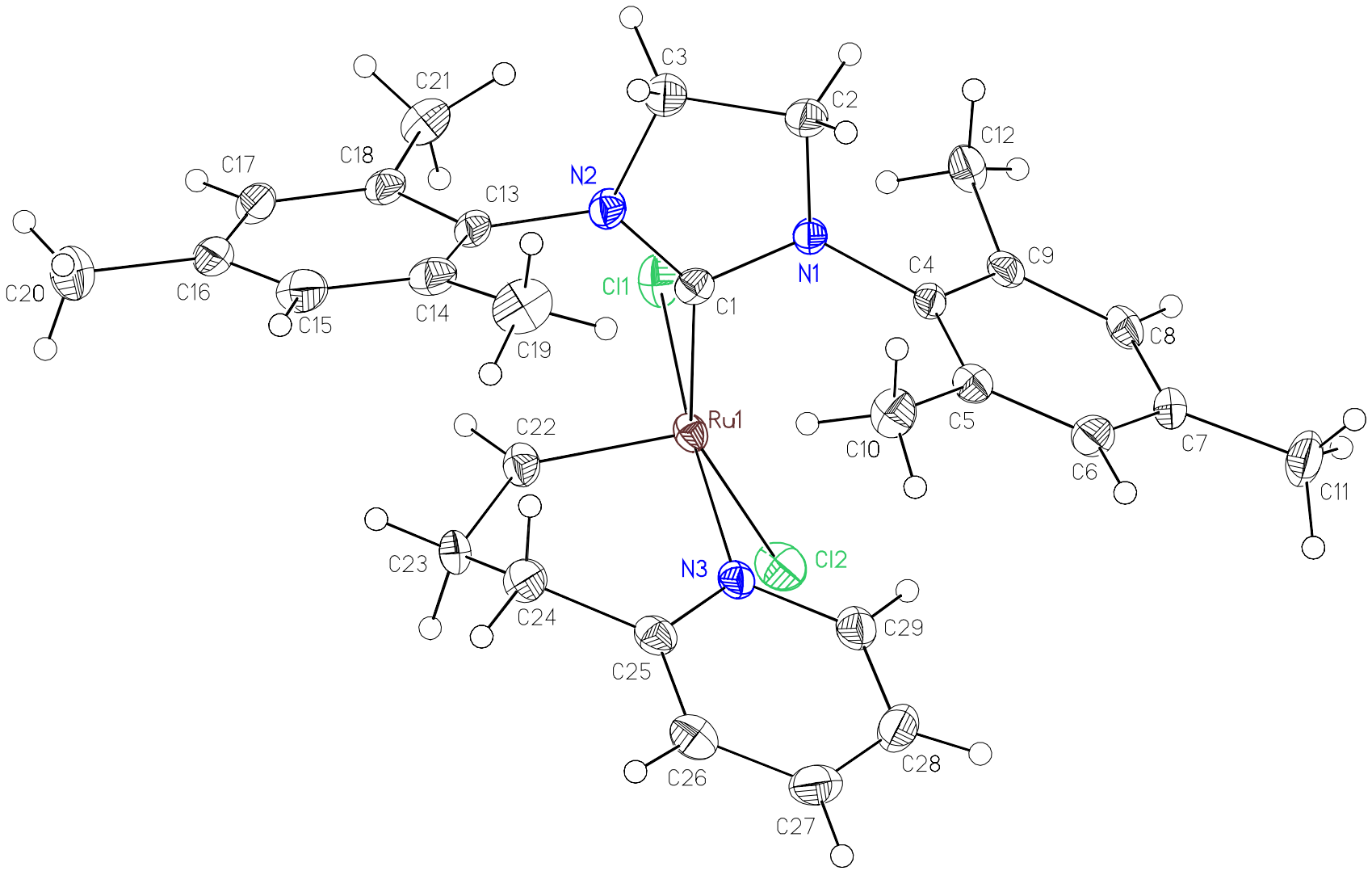
Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	6963 / 0 / 491
Treatment of hydrogen atoms	Unrestrained
Goodness-of-fit on F^2	1.749
Final R indices [$I>2\sigma(I)$, 5556 reflections]	R1 = 0.0347, *w*R2 = 0.0595
R indices (all data)	R1 = 0.0477, *w*R2 = 0.0608
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.035
Average shift/error	0.001
Largest diff. peak and hole	1.224 and -0.983 e.Å^{-3}

Special Refinement Details

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C2
C21
C12
C18
C17
N2
C13
N1
C4
C9
C20
C16
Cl1
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C14
C19
C8
C22
Ru1
C10
C5
C6
C7
C11
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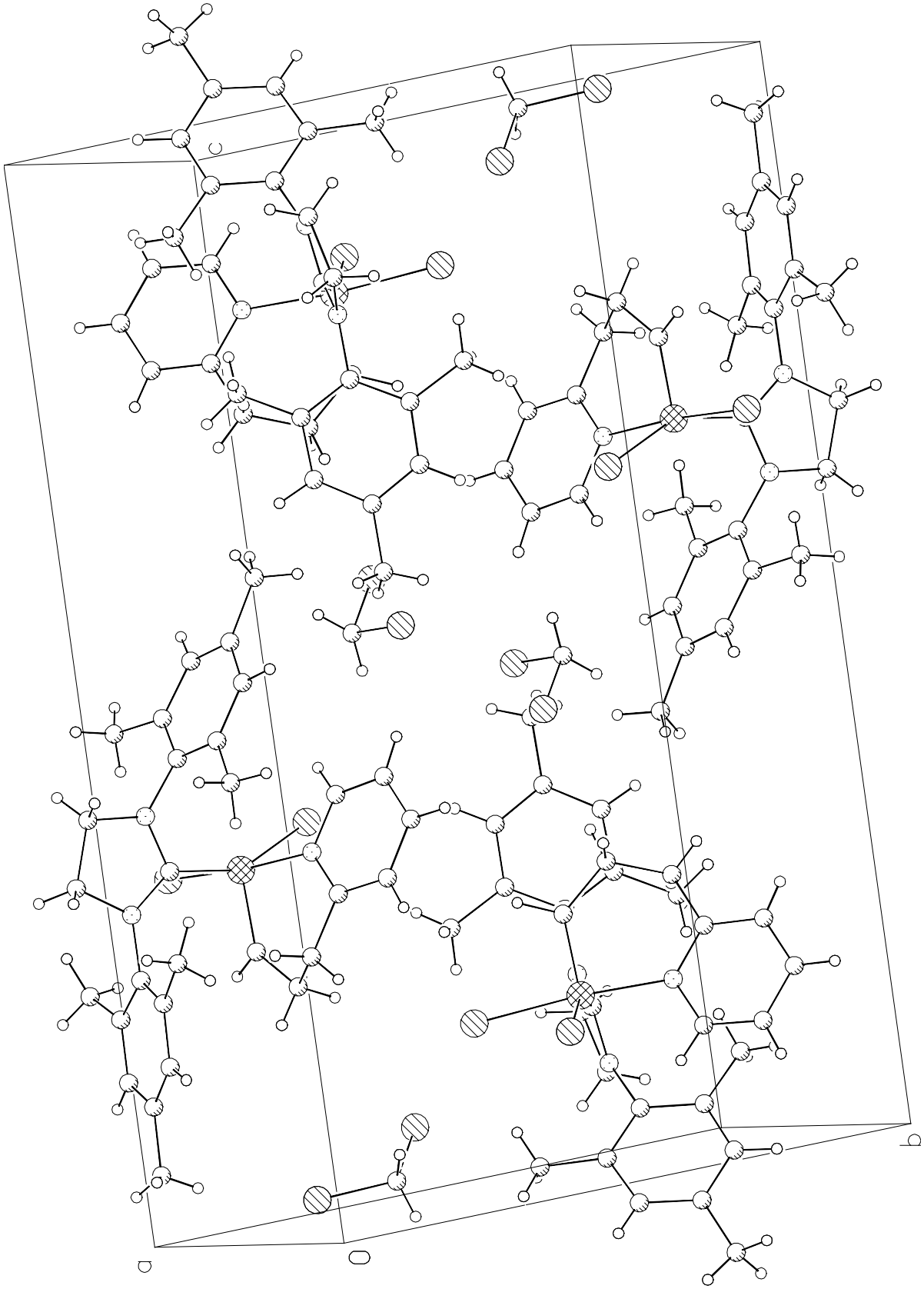
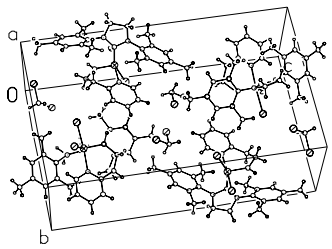
Cl2
C24
C29
C25
C26
C28
C27


c
b


a
0
b

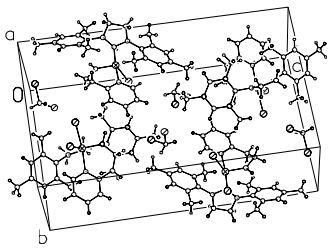

a
0
b

Table 7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 4b. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	4194(1)	6014(1)	1641(1)	15(1)
Cl(1)	5142(1)	4433(1)	1560(1)	23(1)
Cl(2)	6511(1)	6501(1)	1261(1)	26(1)
N(1)	1368(2)	5420(1)	1071(1)	16(1)
N(2)	1157(2)	5018(1)	1936(1)	18(1)
N(3)	3627(2)	7454(1)	1633(1)	17(1)
C(1)	2050(2)	5484(2)	1589(1)	16(1)
C(2)	-65(3)	4891(2)	1042(1)	20(1)
C(3)	-185(3)	4572(2)	1637(1)	24(1)
C(4)	1765(2)	5975(2)	598(1)	16(1)
C(5)	1172(2)	6890(2)	534(1)	17(1)
C(6)	1446(3)	7379(2)	51(1)	22(1)
C(7)	2286(3)	6986(2)	-364(1)	20(1)
C(8)	2854(3)	6087(2)	-286(1)	19(1)
C(9)	2583(3)	5553(2)	185(1)	17(1)
C(10)	227(3)	7331(2)	965(1)	24(1)
C(11)	2468(4)	7503(2)	-904(1)	32(1)
C(12)	3042(3)	4536(2)	217(1)	22(1)
C(13)	1246(2)	4994(2)	2538(1)	17(1)
C(14)	330(3)	5621(2)	2817(1)	22(1)
C(15)	381(3)	5568(2)	3398(1)	27(1)
C(16)	1247(3)	4909(2)	3698(1)	27(1)
C(17)	2076(3)	4268(2)	3408(1)	24(1)
C(18)	2080(3)	4285(2)	2826(1)	18(1)
C(19)	-740(4)	6308(2)	2520(1)	32(1)
C(20)	1254(6)	4876(3)	4329(1)	44(1)
C(21)	2922(3)	3538(2)	2532(1)	26(1)
C(22)	4463(3)	5993(2)	2396(1)	19(1)
C(23)	4109(3)	6742(2)	2800(1)	21(1)
C(24)	2892(3)	7437(2)	2596(1)	23(1)
C(25)	3169(3)	7958(2)	2071(1)	20(1)
C(26)	2916(3)	8919(2)	2029(1)	25(1)
C(27)	3120(3)	9395(2)	1539(1)	28(1)
C(28)	3589(3)	8881(2)	1092(1)	27(1)
C(29)	3833(3)	7933(2)	1153(1)	22(1)
Cl(3)	7775(1)	7780(1)	9166(1)	90(1)
Cl(4)	5536(1)	8901(1)	9705(1)	75(1)
C(30)	6383(5)	7770(3)	9656(2)	62(1)

Table 8. Selected bond lengths [Å] and angles [°] for 4b.

Ru(1)-C(22)	1.811(2)	C(22)-Ru(1)-C(1)	96.67(9)
Ru(1)-C(1)	2.024(2)	C(22)-Ru(1)-N(3)	92.35(10)
Ru(1)-N(3)	2.0977(19)	C(1)-Ru(1)-N(3)	98.04(8)
Ru(1)-Cl(2)	2.3883(6)	C(22)-Ru(1)-Cl(2)	109.21(7)
Ru(1)-Cl(1)	2.4000(6)	C(1)-Ru(1)-Cl(2)	153.74(6)
		N(3)-Ru(1)-Cl(2)	85.63(5)
		C(22)-Ru(1)-Cl(1)	92.44(8)
		C(1)-Ru(1)-Cl(1)	88.62(6)
		N(3)-Ru(1)-Cl(1)	171.29(5)
		Cl(2)-Ru(1)-Cl(1)	85.93(2)

Table 9. Bond lengths [Å] and angles [°] for 4b.

Ru(1)-C(22)	1.811(2)	C(19)-H(19C)	0.95(3)
Ru(1)-C(1)	2.024(2)	C(20)-H(20A)	0.87(3)
Ru(1)-N(3)	2.0977(19)	C(20)-H(20B)	0.90(4)
Ru(1)-Cl(2)	2.3883(6)	C(20)-H(20C)	0.83(3)
Ru(1)-Cl(1)	2.4000(6)	C(21)-H(21A)	0.97(3)
N(1)-C(1)	1.346(3)	C(21)-H(21B)	0.91(3)
N(1)-C(4)	1.443(3)	C(21)-H(21C)	0.89(3)
N(1)-C(2)	1.462(3)	C(22)-C(23)	1.483(3)
N(2)-C(1)	1.352(3)	C(22)-H(22)	1.02(2)
N(2)-C(13)	1.444(3)	C(23)-C(24)	1.512(3)
N(2)-C(3)	1.480(3)	C(23)-H(23A)	0.97(2)
N(3)-C(25)	1.354(3)	C(23)-H(23B)	0.92(2)
N(3)-C(29)	1.358(3)	C(24)-C(25)	1.492(3)
C(2)-C(3)	1.510(3)	C(24)-H(24A)	0.92(2)
C(2)-H(2A)	0.93(2)	C(24)-H(24B)	0.91(2)
C(2)-H(2B)	0.89(2)	C(25)-C(26)	1.381(3)
C(3)-H(3A)	0.93(2)	C(26)-C(27)	1.377(3)
C(3)-H(3B)	0.99(2)	C(26)-H(26)	0.88(2)
C(4)-C(9)	1.397(3)	C(27)-C(28)	1.382(4)
C(4)-C(5)	1.400(3)	C(27)-H(27)	0.95(2)
C(5)-C(6)	1.384(3)	C(28)-C(29)	1.365(4)
C(5)-C(10)	1.504(3)	C(28)-H(28)	0.91(2)
C(6)-C(7)	1.394(3)	C(29)-H(29)	0.92(2)
C(6)-H(6)	0.94(2)	Cl(3)-C(30)	1.752(4)
C(7)-C(8)	1.374(3)	Cl(4)-C(30)	1.771(4)
C(7)-C(11)	1.506(3)	C(30)-H(30A)	0.91(5)
C(8)-C(9)	1.394(3)	C(30)-H(30B)	0.86(4)
C(8)-H(8)	0.86(2)		
C(9)-C(12)	1.495(3)	C(22)-Ru(1)-C(1)	96.67(9)
C(10)-H(10A)	0.87(3)	C(22)-Ru(1)-N(3)	92.35(10)
C(10)-H(10B)	0.94(3)	C(1)-Ru(1)-N(3)	98.04(8)
C(10)-H(10C)	0.91(3)	C(22)-Ru(1)-Cl(2)	109.21(7)
C(11)-H(11A)	0.99(3)	C(1)-Ru(1)-Cl(2)	153.74(6)
C(11)-H(11B)	0.96(3)	N(3)-Ru(1)-Cl(2)	85.63(5)
C(11)-H(11C)	0.98(3)	C(22)-Ru(1)-Cl(1)	92.44(8)
C(12)-H(12A)	0.93(3)	C(1)-Ru(1)-Cl(1)	88.62(6)
C(12)-H(12B)	0.92(3)	N(3)-Ru(1)-Cl(1)	171.29(5)
C(12)-H(12C)	0.89(2)	Cl(2)-Ru(1)-Cl(1)	85.93(2)
C(13)-C(14)	1.397(3)	C(1)-N(1)-C(4)	125.05(18)
C(13)-C(18)	1.398(3)	C(1)-N(1)-C(2)	114.09(18)
C(14)-C(15)	1.395(3)	C(4)-N(1)-C(2)	119.51(17)
C(14)-C(19)	1.500(4)	C(1)-N(2)-C(13)	129.24(19)
C(15)-C(16)	1.376(4)	C(1)-N(2)-C(3)	112.76(18)
C(15)-H(15)	0.93(2)	C(13)-N(2)-C(3)	117.58(18)
C(16)-C(17)	1.380(4)	C(25)-N(3)-C(29)	117.3(2)
C(16)-C(20)	1.515(4)	C(25)-N(3)-Ru(1)	125.93(15)
C(17)-C(18)	1.397(3)	C(29)-N(3)-Ru(1)	116.65(16)
C(17)-H(17)	0.95(2)	N(1)-C(1)-N(2)	107.12(19)
C(18)-C(21)	1.493(4)	N(1)-C(1)-Ru(1)	115.98(15)
C(19)-H(19A)	0.84(3)	N(2)-C(1)-Ru(1)	135.86(16)
C(19)-H(19B)	0.96(3)	N(1)-C(2)-C(3)	102.77(19)

N(1)-C(2)-H(2A)	110.2(15)	C(16)-C(15)-H(15)	123.0(15)
C(3)-C(2)-H(2A)	115.1(15)	C(14)-C(15)-H(15)	114.3(15)
N(1)-C(2)-H(2B)	107.6(14)	C(15)-C(16)-C(17)	118.3(2)
C(3)-C(2)-H(2B)	112.5(14)	C(15)-C(16)-C(20)	120.6(3)
H(2A)-C(2)-H(2B)	108(2)	C(17)-C(16)-C(20)	121.1(3)
N(2)-C(3)-C(2)	103.10(19)	C(16)-C(17)-C(18)	122.0(2)
N(2)-C(3)-H(3A)	108.9(15)	C(16)-C(17)-H(17)	119.8(13)
C(2)-C(3)-H(3A)	114.6(15)	C(18)-C(17)-H(17)	118.1(13)
N(2)-C(3)-H(3B)	109.2(13)	C(13)-C(18)-C(17)	118.0(2)
C(2)-C(3)-H(3B)	116.0(13)	C(13)-C(18)-C(21)	122.4(2)
H(3A)-C(3)-H(3B)	105(2)	C(17)-C(18)-C(21)	119.6(2)
C(9)-C(4)-C(5)	121.6(2)	C(14)-C(19)-H(19A)	111.4(19)
C(9)-C(4)-N(1)	119.2(2)	C(14)-C(19)-H(19B)	111.5(15)
C(5)-C(4)-N(1)	118.84(19)	H(19A)-C(19)-H(19B)	107(2)
C(6)-C(5)-C(4)	118.0(2)	C(14)-C(19)-H(19C)	111.1(17)
C(6)-C(5)-C(10)	120.2(2)	H(19A)-C(19)-H(19C)	106(3)
C(4)-C(5)-C(10)	121.7(2)	H(19B)-C(19)-H(19C)	110(2)
C(5)-C(6)-C(7)	121.8(2)	C(16)-C(20)-H(20A)	112(2)
C(5)-C(6)-H(6)	121.0(14)	C(16)-C(20)-H(20B)	112(2)
C(7)-C(6)-H(6)	117.2(14)	H(20A)-C(20)-H(20B)	102(3)
C(8)-C(7)-C(6)	118.6(2)	C(16)-C(20)-H(20C)	106(2)
C(8)-C(7)-C(11)	120.6(2)	H(20A)-C(20)-H(20C)	109(3)
C(6)-C(7)-C(11)	120.7(2)	H(20B)-C(20)-H(20C)	116(3)
C(7)-C(8)-C(9)	122.1(2)	C(18)-C(21)-H(21A)	113.8(15)
C(7)-C(8)-H(8)	120.9(15)	C(18)-C(21)-H(21B)	110.5(16)
C(9)-C(8)-H(8)	116.8(15)	H(21A)-C(21)-H(21B)	106(2)
C(8)-C(9)-C(4)	117.8(2)	C(18)-C(21)-H(21C)	110.9(17)
C(8)-C(9)-C(12)	120.3(2)	H(21A)-C(21)-H(21C)	106(2)
C(4)-C(9)-C(12)	121.7(2)	H(21B)-C(21)-H(21C)	109(2)
C(5)-C(10)-H(10A)	110(2)	C(23)-C(22)-Ru(1)	128.50(19)
C(5)-C(10)-H(10B)	109.9(17)	C(23)-C(22)-H(22)	115.2(12)
H(10A)-C(10)-H(10B)	104(2)	Ru(1)-C(22)-H(22)	116.0(12)
C(5)-C(10)-H(10C)	111.3(18)	C(22)-C(23)-C(24)	115.3(2)
H(10A)-C(10)-H(10C)	114(3)	C(22)-C(23)-H(23A)	108.7(14)
H(10B)-C(10)-H(10C)	108(2)	C(24)-C(23)-H(23A)	113.4(14)
C(7)-C(11)-H(11A)	111.7(16)	C(22)-C(23)-H(23B)	108.3(14)
C(7)-C(11)-H(11B)	115.1(15)	C(24)-C(23)-H(23B)	110.1(14)
H(11A)-C(11)-H(11B)	105(2)	H(23A)-C(23)-H(23B)	99.7(18)
C(7)-C(11)-H(11C)	108.5(18)	C(25)-C(24)-C(23)	116.3(2)
H(11A)-C(11)-H(11C)	114(2)	C(25)-C(24)-H(24A)	109.0(14)
H(11B)-C(11)-H(11C)	102(2)	C(23)-C(24)-H(24A)	107.8(14)
C(9)-C(12)-H(12A)	108.3(16)	C(25)-C(24)-H(24B)	105.4(15)
C(9)-C(12)-H(12B)	112.1(17)	C(23)-C(24)-H(24B)	111.8(15)
H(12A)-C(12)-H(12B)	112(2)	H(24A)-C(24)-H(24B)	106(2)
C(9)-C(12)-H(12C)	111.2(16)	N(3)-C(25)-C(26)	121.1(2)
H(12A)-C(12)-H(12C)	109(2)	N(3)-C(25)-C(24)	118.0(2)
H(12B)-C(12)-H(12C)	104(2)	C(26)-C(25)-C(24)	120.9(2)
C(14)-C(13)-C(18)	121.3(2)	C(27)-C(26)-C(25)	121.0(2)
C(14)-C(13)-N(2)	118.0(2)	C(27)-C(26)-H(26)	122.6(16)
C(18)-C(13)-N(2)	120.2(2)	C(25)-C(26)-H(26)	116.3(16)
C(15)-C(14)-C(13)	117.6(2)	C(26)-C(27)-C(28)	117.9(3)
C(15)-C(14)-C(19)	119.2(2)	C(26)-C(27)-H(27)	121.6(13)
C(13)-C(14)-C(19)	123.2(2)	C(28)-C(27)-H(27)	120.5(13)
C(16)-C(15)-C(14)	122.6(2)	C(29)-C(28)-C(27)	119.1(2)

C(29)-C(28)-H(28)	118.9(15)
C(27)-C(28)-H(28)	122.1(15)
N(3)-C(29)-C(28)	123.6(2)
N(3)-C(29)-H(29)	115.2(14)
C(28)-C(29)-H(29)	121.2(14)
Cl(3)-C(30)-Cl(4)	110.6(2)
Cl(3)-C(30)-H(30A)	107(4)
Cl(4)-C(30)-H(30A)	103(3)
Cl(3)-C(30)-H(30B)	94(3)
Cl(4)-C(30)-H(30B)	105(3)
H(30A)-C(30)-H(30B)	136(4)

Table 10. Anisotropic displacement parameters ($Å^2 x 10^4$) for 4b. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	123(1)	200(1)	123(1)	-19(1)	16(1)	-7(1)
Cl(1)	236(3)	266(3)	186(3)	-7(2)	31(2)	79(3)
Cl(2)	171(3)	360(4)	269(3)	-63(3)	79(2)	-53(3)
N(1)	142(10)	190(11)	134(9)	20(8)	-3(8)	-41(8)
N(2)	146(10)	220(11)	159(10)	25(8)	11(8)	-27(9)
N(3)	137(10)	220(11)	148(9)	-4(8)	0(8)	-41(8)
C(1)	170(12)	113(12)	185(12)	-3(9)	20(9)	35(10)
C(2)	171(13)	218(15)	220(13)	16(11)	-4(11)	-50(11)
C(3)	182(14)	322(17)	225(13)	41(12)	-13(11)	-105(12)
C(4)	126(11)	207(13)	129(10)	22(10)	-16(8)	-46(10)
C(5)	145(12)	198(13)	179(12)	-18(10)	12(9)	-2(10)
C(6)	249(14)	165(14)	231(13)	12(10)	-22(11)	20(11)
C(7)	269(14)	206(14)	128(11)	11(10)	0(10)	-23(11)
C(8)	194(12)	241(14)	135(11)	-51(11)	18(9)	3(11)
C(9)	147(12)	190(13)	159(11)	-19(10)	-35(9)	-20(10)
C(10)	233(15)	254(17)	236(15)	-6(12)	77(12)	36(13)
C(11)	530(20)	265(17)	172(13)	51(12)	84(14)	25(15)
C(12)	253(15)	229(15)	161(13)	-19(11)	-8(12)	49(12)
C(13)	143(12)	202(13)	162(12)	26(10)	33(9)	-45(10)
C(14)	193(13)	201(13)	269(13)	0(11)	56(10)	-46(11)
C(15)	304(15)	238(15)	276(14)	-55(12)	142(12)	-51(12)
C(16)	364(16)	261(15)	185(13)	-1(11)	64(11)	-134(13)
C(17)	264(14)	234(15)	222(13)	74(11)	-27(11)	-74(11)
C(18)	159(12)	186(13)	205(12)	27(10)	31(10)	-48(10)
C(19)	246(17)	306(18)	427(18)	29(14)	68(14)	56(13)
C(20)	730(30)	410(20)	196(15)	-33(15)	78(17)	-170(20)
C(21)	252(16)	212(15)	305(15)	54(12)	53(12)	15(13)
C(22)	154(12)	259(14)	157(11)	13(11)	13(9)	-15(12)
C(23)	286(15)	244(15)	114(12)	4(10)	14(11)	-35(12)
C(24)	300(16)	197(15)	198(13)	-38(11)	94(11)	1(12)
C(25)	155(12)	227(14)	202(12)	-28(10)	3(10)	-27(10)
C(26)	257(14)	251(15)	248(13)	-58(12)	2(11)	3(12)
C(27)	286(15)	200(15)	356(16)	17(12)	-29(12)	-41(12)
C(28)	265(14)	313(16)	236(13)	94(12)	-22(11)	-66(12)
C(29)	188(13)	276(15)	181(12)	-5(11)	11(10)	-45(11)
Cl(3)	772(7)	598(7)	1382(10)	402(6)	516(7)	12(5)
Cl(4)	689(6)	294(5)	1275(9)	49(5)	120(6)	-4(4)
C(30)	460(20)	320(20)	1080(40)	120(20)	150(30)	22(18)

Table 11. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 4b.

	x	y	z	U_{iso}
H(2A)	-30(30)	4409(18)	782(10)	27(7)
H(2B)	-810(30)	5289(16)	928(9)	11(6)
H(3A)	-1060(30)	4773(17)	1800(10)	25(7)
H(3B)	-150(30)	3881(17)	1701(9)	21(6)
H(6)	1080(30)	7998(17)	-7(9)	23(7)
H(8)	3350(20)	5817(15)	-538(9)	11(6)
H(10A)	290(30)	7950(20)	947(12)	57(10)
H(10B)	650(30)	7180(20)	1327(12)	46(9)
H(10C)	-750(30)	7110(20)	936(11)	46(9)
H(11A)	3260(30)	7211(19)	-1122(11)	45(8)
H(11B)	2770(30)	8152(19)	-864(10)	30(7)
H(11C)	1460(40)	7550(20)	-1107(13)	65(10)
H(12A)	2170(30)	4168(18)	155(10)	35(8)
H(12B)	3560(30)	4392(19)	551(11)	43(8)
H(12C)	3700(30)	4396(17)	-39(10)	24(7)
H(15)	-230(30)	6012(17)	3566(10)	28(7)
H(17)	2690(30)	3815(16)	3605(9)	18(6)
H(19A)	-1620(30)	6080(20)	2464(11)	38(9)
H(19B)	-390(30)	6484(18)	2161(11)	33(8)
H(19C)	-860(30)	6860(20)	2739(12)	51(9)
H(20A)	1950(40)	5250(20)	4488(13)	57(11)
H(20B)	1540(40)	4310(30)	4467(14)	79(13)
H(20C)	400(40)	5060(20)	4409(14)	62(13)
H(21A)	2460(30)	3379(18)	2165(11)	36(8)
H(21B)	2960(30)	2994(19)	2733(10)	31(7)
H(21C)	3870(30)	3724(18)	2478(10)	33(8)
H(22)	5030(30)	5421(16)	2565(9)	22(6)
H(23A)	5050(30)	7041(17)	2936(9)	22(7)
H(23B)	3840(20)	6458(16)	3123(9)	16(6)
H(24A)	1980(30)	7113(16)	2547(9)	16(6)
H(24B)	2740(30)	7891(17)	2854(10)	24(7)
H(26)	2680(30)	9206(17)	2334(9)	22(7)
H(27)	2970(20)	10055(16)	1509(8)	11(6)
H(28)	3710(30)	9151(16)	755(10)	25(7)
H(29)	4180(30)	7577(16)	869(9)	15(6)
H(30A)	6880(60)	7690(40)	10000(20)	160(30)
H(30B)	5730(40)	7450(30)	9447(15)	75(14)